2-Hydroxyphenylacetic acid								
	614-75-5 DTXSID1060633							

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 261 °C

Global applicability domain: Inside

Local applicability domain index: 2.55e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

Image not found

2-Hydroxyphenylacetic acid

Measured: 240 Predicted: 261

Image not found

2-Chlorobenzoic acid

Measured: 287 Predicted: 273

Image not found

2,5-Dichlorobenzoic acid

Measured: 301 Predicted: 288

Image not found

Benzoic acid, 4-methoxy-

Measured: 277 Predicted: 279